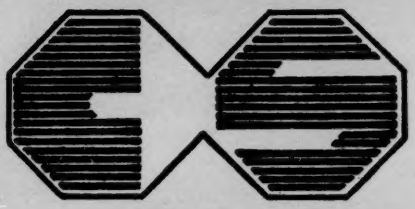

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THE SEVENTH ANNUAL GENERAL MEETING OF THE FARADAY DIVISION of The Chemical Society was held at 9.00 a.m., on 14 September 1978, in the Physics Lecture Theatre, The University, Canterbury with Professor F. C. Tompkins D.Sc., C.Chem., F.R.I.C., F.R.S. in the Chair.

1 *Minutes*

The President commenced by reporting that the Minutes of the 6th Annual General Meeting were to be published in the index to the 1977 Farady Transactions which was not yet in print but which would appear in due course. The Minutes, which had therefore been tabled, were confirmed.

2 *Annual Report*

In 1977, Professor F. C. Tompkins retired after 30 years as Editor of the Faraday Transactions. To mark this event and also his impending retirement as Honorary Secretary of the Faraday Society and Division after a similar period, members contributed towards a gift of Bristol crystal. The decanter and glasses, together with a cheque and a book containing the signatures of those who had contributed, were presented to Professor Tompkins by the President before a gathering of Council members and past Presidents. Dr. D. A. Young took over the post of Scientific Editor of the Faraday Transactions in August 1977.

Two General Discussions were held in 1977. In March, Discussion 63 'Radiation Effects in Liquids and Solids' was held in Leicester when 120 persons attended of whom over 70 were from overseas. The second, Discussion No. 64 'Ion–Ion and Ion–Solvent Interactions' was held at St. Catherine's College, Oxford in September and attracted nearly 200 participants of whom half were from overseas representing 19 countries. This Discussion marked the 20th anniversary of the meeting on 'Interactions in Ionic Solutions' and the 50th anniversary of the meeting on 'The Theory of Strong Electrolytes' and the Division welcomed 5 of the participants in the 1927 Discussion as guests at the Dinner. For the first time at a Faraday Discussion, a poster session was held which allowed the presentation of contributions which were not for publication in the Discussion proceedings.

The Symposium in 1977 was held in Southampton in December on 'Electrocrystallization, Nucleation and Phase Formation' which attracted 100 participants of whom one third were from overseas.

The Faraday contribution to the Annual Congress held at University College London, comprised an informal discussion on 'Pair Interactions between Molecules' and at the Autumn Meeting in Aberdeen an informal discussion on 'The Chemistry of the Atmosphere'. An informal meeting on 'High Resolution Laser Spectroscopy' was held in Cambridge in December which led to the formation of a new subject group for High Resolution Spectroscopy.

Collaboration with the Institute of Physics was maintained in 1977 with the co-sponsorship of two meetings, 'The 3rd National Quantum Electronics Conference' and 'The 50th Anniversary of Electron Diffraction'.

Group meetings again played an important part in the activities of the Division and included the following topics:

Molecular Beam Kinetics (Molecular Beams Group)
Competing Channels in Elementary Processes (Gas Kinetics Group)
The Nature of the Glass Transition in Polymers (Polymer Physics Group)
Quantum Theory of Chemical Dynamics (Theoretical Chemistry Group)
Polymer Surfaces (Polymer Physics Group)
3rd Interdisciplinary Surface Science Conference (Surface Reactivity and Catalysis Group)
Hot Neutron Scattering (Neutron Scattering Group)
Mechanism of Environmental Corrosion Cracking (Electrochemistry Group)
Fundamental Electrochemistry (Electrochemistry Group)
6th Polymer Meeting Point (Polymer Physics Group)
Lipid Bilayers: Structure, Dynamics and Interactions with Small Molecules (Colloid and Interface Science Group)

Low Angle Neutron Scattering from Polymers (Neutron Scattering Group)
Advanced Instrumental Methods in Electrode Kinetics (Electrochemistry Group)
5th International Symposium on Gas Kinetics (Gas Kinetics Group)
Processing, Structure, Properties and Performance of Polymers (Polymer Physics Group)
4th European Crystallography Meeting (Polymer Physics Group)
Experimental Neutron Scattering (Neutron Scattering Group)
Surface Phenomena in Analysis (Electrochemistry Group)
General Aspects of Chemisorption and Catalysis (Surface Reactivity and Catalysis Group)
Statistical and Dynamic Behaviour of Chain Molecules (Statistical Mechanics and Thermodynamics Group)
Concentrated Dispersions (Industrial Sub-Committee with Colloid and Interface Science Group)
High Temperature Battery Systems (Electrochemistry Group)
Molecular Beams in Combustion Research (Molecular Beams Group)
Polymer Materials at Low Temperatures (Polymer Physics Group)
Molecules Adsorbed at Surfaces (Theoretical Chemistry Group)
Magnetism Density Distribution (Neutron Scattering Group)

The 1977 Bourke Lecturer was Professor R. G. Gordon of Harvard University who lectured on 'Molecular Dynamics of Collisions', 'Solid State Chemistry' and 'Intermolecular Forces' at the University of Strathclyde, University College of Wales, Aberystwyth and the University of Bristol respectively. A London Symposium on 'Molecular Beams in Chemistry' was sponsored by the Faraday Division which incorporated the Centenary Lecture of Professor D. R. Herschbach. Dr. J. N. L. Connor (University of Manchester), distinguished for his contributions to the understanding of scattering processes in gases, was awarded the 1977 Marlow Medal.

Regular communication with members was continued with the distribution in February of Newsletter No. 4. The total number of members of the Division in 1977 was 4414, there having been a small increase in the number of overseas members during the year.

Professor Tompkins thanked members for the gift made to him on his retirement as Editor and Secretary.

3 *Treasurer's Report*

The Treasuer reported that it had been possible to increase further the support to scientific meetings and in 1979 the maximum sums available would be:

General Discussions	£720
Symposium	£500
Annual Congress	£250
Autumn Meeting	£250

As from 1978 Divisions would carry forward to the following year the whole of any unspent balances accruing at the end of the year.

The Society was in the process of changing its financial year from the academic to the calendar year and as a result the 1977–8 accounting period was 15 months ending in December 1978.

4 *Elections to Council*

The President announced that the postal ballot for Ordinary Members of Council, conducted among members of the Division, had resulted in the following two persons being elected: Professor D. A. King and Professor J. H. Purnell.
The members of Council of the Faraday Division of the Chemical Society to take office from July 1979 were as follows:

President

PROF. J. S. ROWLINSON

Vice-Presidents who have held office as President

PROF. SIR GEORGE PORTER
DR. T. M. SUGDEN
PROF. R. P. BELL
PROF. D. H. EVERETT
PROF. F. C. TOMPKINS

Vice-Presidents

PROF. A. D. BUCKINGHAM
PROF. P. GRAY
PROF. G. J. HILLS
PROF. N. SHEPPARD
DR. H. A. SKINNER
PROF. J. G. WAGNER
PROF. D. H. WHIFFEN

Ordinary Members

PROF. W. J. ALBERY
PROF. J. H. BAXENDALE
PROF. F. FRANKS
PROF. D. A. KING
PROF. G. R. LUCKHURST
PROF. P. MEARES
PROF. J. H. PURNELL
DR. J. P. SIMONS
PROF. F. S. STONE
DR. D. A. YOUNG

Honorary Treasurer

PROF. P. GRAY

Honorary Secretary

PROF. G. J. HILLS

The President thanked the retiring members for their services: Professor G. Gee, Dr. W. J. Dunning and Professor B. A. Thrush.

The President paid tribute to Professor R. G. W. Norrish, past President of the Faraday Society, and to Professor M. Magat, Vice-President of the Faraday Division, both ardent supporters of the Society who had died in 1978.

5 *Review of Future Activities*

The President drew attention to the programme of future activities of the Division which had been tabled. Two further meetings in the series with the Société de Chimie Physique, Deutsche Bunsen Gesellschaft and Associazione Italiana di Chimica Fisica were planned, the first to be heid in Fontevraud, France in September 1978 and the second in Italy in 1980. Arrangements for the 1978 General Discussions on 'Kinetics of State Selected Species' to be held in April in Birmingham and on 'Organization of Macromolecules in the Condensed Phase' to be held in Cambridge in September were well advanced and the topics for the 1980 General Discussions had been chosen: 'Phase Transitions in Molecular Solids' in the spring and 'Photoelectrochemistry' in September. The 1979 Bourke Lecturer was Professor O. Kedem of the Weizmann Institute, Israel.

6 *Unification*

The President informed members that the Faraday Division was satisfied with the unification proposals and urged all members to take advantage of the facility to vote by proxy.

NOTICES TO AUTHORS—No. 7/1970

Deposition of Data—Supplementary Publications Scheme

Preamble

The growing volume of research that produces large quantities of data, the increasing facilities for analysing such data mechanically, and the rising cost of printing are each making it very difficult to publish in the *Journal* in the normal way the full details of the experimental data which become available. Moreover, whilst there is a large audience for the general method and conclusions of a research project, the number of scientists interested in the details, and in particular in the data, of any particular case may be quite small. The British Library Lending Division (B.L.L.D.) in consultation with the Editors of scientific journals, has now developed a scheme whereby such data and detail may be stored and then copies made available on request at the B.L.L.D., Boston Spa. The Chemical Society is a sponsor of this scheme and has indicated to the B.L.L.D. its wish to use the facilities being made available in this "Supplementary Publications Scheme".

Bulk information (such as crystallographic structure factor tables, computer programmes and output, evidence for amino-acid sequences, spectra, *etc.*), which accompany papers published in future issues of the Chemical Society's *Journal* may in future be deposited, free of charge, with the Supplementary Publications Scheme, either at the request of the author and with the approval of the referees or on the recommendation of referees and the approval of the author.

The Scheme

Under this scheme, authors will submit articles and the supplementary material to the *Journal* simultaneously in the normal way, and both will be refereed. If the paper is accepted for publication the supplementary material will be sent by the Society to the B.L.L.D. where it will be stored. Copies will be obtainable by individuals both in the U.K. and abroad on quoting a supplementary publication number that will appear in the parent article.

Preparation of Material

Authors will be responsible for the preparation of camera-ready copy according to the following specifications (although the Society will be prepared to help in case of difficulty).

(*a*) Optimum page size for text or tables in typescript: up to 30 cm × 21 cm.

(*b*) Limiting page size for text or tables in typescript: 33 cm × 24 cm.

(*c*) Limiting size for diagrams, graphs, spectra, *etc.*: 39 cm × 28·5 cm.

(*d*) Tabular matter should be headed descriptively on the first page, with column headings recurring on each page.

(*e*) Pages should be clearly numbered.

It is recommended that all material which is to be deposited should be accompanied by some prefatory text. Normally this will be the summary from the parent paper and authors will greatly aid the deposition of the material if a duplicate copy of the summary is provided. If authors have the facilities available the use of a type face designed to be read by computers is encouraged.

Deposition

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Action by the Society

The Society will receive a manuscript for publication together with any supplementary material for deposition and will circulate all of this to referees in the normal way. When the edited manuscript is sent to the printers the supplementary material will be sent for deposition to the B.L.L.D. who will issue the necessary publication number. The Society will add to the paper, at the galley proof stage, a footnote indicating what material has been deposited in the Supplementary Publications Scheme, the number of pages it occupies, the supplementary publication number, and details as to how copies may be obtained.

Availability

Copies of Supplementary Publications may be obtained from the B.L.L.D. on demand by organisations which are registered borrowers. They should use the normal forms and coupons for such requests addressing them as follows:

Mr. J. P. Chillag,
British Library Lending Division,
Boston Spa,
Wetherby,
West Yorkshire, LS23 7BQ, U.K.

Non-registered users may also obtain copies of Supplementary Publications but should first apply for price quotations. These are available from the Loans Office at the above address.

In all correspondence with the B.L.L.D. or the Society authors must cite the supplementary publication number.

International Collaboration

A similar scheme (known as the National Auxiliary Publications Service) is being operated in the U.S.A. by the American Society for Information Science. Similar schemes are also being contemplated in other countries. The provision of reciprocal arrangements for the exchange of supplementary data between the various national deposition centres is being investigated.

NOTICE TO AUTHORS—No. 9/1974

Nomenclature

For many years the Society has actively encouraged the use of standard I.U.P.A.C. nomenclature and symbolism in its publications as an aid to the accurate and unambiguous communication of chemical information between authors and readers. Although the I.U.P.A.C. rules for naming organic compounds have now gained wide acceptance amongst chemists, mainly because they have been in existence for a number of years, those for naming inorganic compounds are of more recent origin and for this reason their acceptance is less general.

In order to encourage authors to use I.U.P.A.C. nomenclature rules when drafting papers, attention is drawn to the following publications in which both the rules themselves and guidance on their use are given.

'Nomenclature of Organic Chemistry, Sections A, B, and C', Butterworths, London, 2nd Edition, 1971.

'Nomenclature of Inorganic Chemistry', Butterworths, London, 1971.

'Manual of Symbols and Terminology for Physicochemical Quantities and Units', Butterworths, London, 1970.

In addition to the above publications, provisional rules for the naming of organometallic compounds, amino-acids, carbohydrates, carotenoids and steroids, and rules of stereochemistry are available from the:

I.U.P.A.C. Secretariat,
Bank Court Chambers,
2-3 Pound Way,
Cowley Centre,
OXFORD OX4 3YF.

It is recommended that where there are no I.U.P.A.C. rules for the naming of particular compounds or authors find difficulty in applying the existing rules, they should seek the advice of the Society's editorial staff.

NOTICE TO AUTHORS—No. 10/1976

Authentication of New Compounds

(1) It is the responsibility of authors to provide fully convincing evidence for the homogeneity and identity of all compounds they claim as new. Evidence of both purity and identity is required to establish that the properties and constants reported are those of the compound with the new structure claimed.

(2) In the context of this Notice a compound is considered as new (*a*) if it has not been prepared before, (*b*) if it has been prepared before but not adequately purified, (*c*) if it has been purified but not adequately characterised, (*d*) if, earlier, it has been assigned an erroneous constitution, or (*e*) if it is a natural product synthesised for the first time. In preliminary communications compounds are often recorded with limited characterising data; in spite of (*c*) above later preparations of such compounds are not considered as new if the properties previously reported are confirmed; the same applies to patents.*

(3) Referees are asked to assess, as a whole, the evidence in support of the homogeneity and structure of all new compounds. No hard and fast rules can be laid down to cover all types of compounds, but the Society's policy remains unchanged in that evidence for the unequivocal identification of new compounds should normally include good elemental analytical data; an accurate mass measurement of a molecular ion does not provide evidence of purity of a compound and must be accompanied by independent evidence of homogeneity. Low-resolution mass spectroscopy must be treated with even more reserve in the absence of firm evidence to distinguish between alternative molecular formulae. Where elemental analytical data are not available, appropriate evidence which is convincing to an expert in the field will be acceptable, but authors should include, for the referees, a brief explanation of the special nature of their problem.

(4) Spectroscopic information necessary to the assignment of structure should normally be given. Just how complete this information should be must depend upon the circumstances; the structure of a compound obtained from an unusual reaction or isolated from a natural source needs much stronger supporting evidence than one derived by a standard reaction from a precursor of undisputed structure. Authors are reminded that full spectroscopic assignments may always be treated as a Supplementary Publication where their importance does not justify their inclusion in the published paper.

(5) Finally, referees are reminded of the need to be exacting in their standards but at the same time flexible in their admission of evidence. It remains the Society's policy to accept work only of high quality and to permit no lowering of present standards.

* New compounds should be indicated by underlining the name (for italics) at its first mention (excluding headings) in the Experimental section only, and by giving analytical results in the form: (Found: C, 63.1; H, 5.4. $C_{13}H_{13}NO_4$ requires C, 63.2; H, 5.3 %). If analytical results for compounds which have been adequately described in the literature are to be included, they should be given in the form: (Found: C, 62.95; H, 5.4. Calc. for $C_{13}H_{13}NO_4$: C, 63.2; H, 5.3 %). Analyses are normally quoted to the nearest 0.05 %.

Publication of Theoretical and Computational Papers

The Primary Journals Committee has been considering future policy towards the publication of papers with a heavily computational content, particularly where these involve standard methods, such as semi-empirical or *ab initio* calculations of molecular electronic properties using readily available computer programs. Many such papers report what would be considered 'routine work' in other areas of chemistry and have often included extensive detail.

A specialist sub-committee formulated a set of proposals which were circulated to a large representative sample of theoretical chemists and met with general acceptance. These, with the comments on them, form the basis of this notice.

The Primary Journals Committee recognises that computational work can play a valuable role in chemistry, and will probably continue to do so on an increasing scale. It accepts the time-honoured principle that the first criterion for publication of a paper by the Society should be the worthiness of the chemical problem considered, rather than the particular techniques employed by the author. For example, the use of a new computing algorithm, or the modification of a program, would not usually, on its own, provide sufficient justification for publication.

The Primary Journals Committee recommends to authors the following guidelines for the preparation of computational papers, so that the material can be presented concisely and effectively.

(i) Papers should be submitted to the appropriate journal: a paper containing innovations in theory to Faraday Transactions II, one in which the computations are incidental to the chemistry to Perkin, Dalton or Faraday I Transactions. Papers concerned mainly with computational details are unlikely to be accepted.

(ii) The purpose of the paper and the precise objectives of the calculations performed should be clearly stated: the results obtained should be reported only in so far as they relate to those objectives.

(iii) Many papers use a routine procedure based on a well documented method, be it semi-empirical or *ab initio*. It is then sufficient to name the particular variant, referring to key papers in which the method was developed, to cite the computer program used, and to indicate *briefly* any modification made by the author. A review of theoretical background would be out of place, but an author should say why he considers the method adequate for his purposes.

(iv) Extensive tabulation of numerical results, such as the magnitudes of atomic orbital coefficients, electron populations, contour maps of molecular orbitals and electron densities, and peripheral material of a similar nature, is normally unnecessary. Lengthy line-by-line discussion of such material is, as a general rule, quite unacceptable. Where an author considers that there is a special need to make such material available to other workers, as with highly accurate computations, for example, then this may be deposited with the British Library as a Supplementary Publication. Such material should be submitted with the main paper, clearly distinguished from it, and referred to in the main text.

Guidelines can never provide sufficient criteria for acceptance or rejection of a paper. Critical assessment of the theoretical methods used in a computation, and of their suitability for the purpose in hand, will continue to be entrusted to specialist referees who must also decide whether the results are new and advance science.

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